STIC Search Report
EIC 1700

STIC Database Tracking Number: 182904

TO: Eisa Elhilo **Location: REM 9A60** **Art Unit : 1751** **March 22, 2006** **Case Serial Number: 10/798454**	**From: Les Henderson** **Location: EIC 1700** **REM 4B28 / 4A30** **Phone: 571-272-2538** **Leslie.henderson@uspto.gov**

Search Notes

STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact ***the EIC searcher or contact:***

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1713*
- *Relevant prior art* ***found****, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art* ***not found:***
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28

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=> d his

     (FILE 'HOME' ENTERED AT 13:19:22 ON 22 MAR 2006)

     FILE 'HCAPLUS' ENTERED AT 13:20:34 ON 22 MAR 2006
                E US20050081313/PN
L1            1 S US20050081313/PN
                SEL RN

     FILE 'REGISTRY' ENTERED AT 13:21:54 ON 22 MAR 2006
L2           53 S E1-E53

     FILE 'LREGISTRY' ENTERED AT 13:25:58 ON 22 MAR 2006
L3              STR

     FILE 'REGISTRY' ENTERED AT 13:36:05 ON 22 MAR 2006
L4            0 S L3
L5              SCR 2043
L7            0 S L3 NOT L5 FUL

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L9              STR L8

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L10           0 S L9
L11           0 S L9 NOT L5

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L12             STR L9

     FILE 'REGISTRY' ENTERED AT 14:05:10 ON 22 MAR 2006
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L14         102 S L12 FUL
                SAV L14 LEE454/A
L15          39 S L14 AND L2

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L16             STR L12

     FILE 'REGISTRY' ENTERED AT 14:12:36 ON 22 MAR 2006
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L18          85 S L16 SSS FUL SUB=L14
                SAV L18 LEE454A/A
L19             STR L16

     FILE 'REGISTRY' ENTERED AT 14:15:33 ON 22 MAR 2006
L20           1 S L19 SSS SAM SUB=L14
L21          53 S L19 SSS FUL SUB=L14
                SAV L21 LEE454B/A
L22          24 S L21 AND L2
L23          39 S L18 AND L2

     FILE 'HCAPLUS' ENTERED AT 14:17:49 ON 22 MAR 2006
L24           7 S L23
L25           2 S L22
L26          13 S L21
L27          24 S L18
L28          28 S L14
L29           7 S L24 OR L15
L30           1 S L1 AND L26
L31          15 S L28 NOT L26

=> d que stat l26
L12             STR
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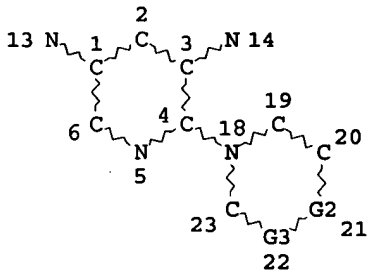

VAR G2=C/N/O
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NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
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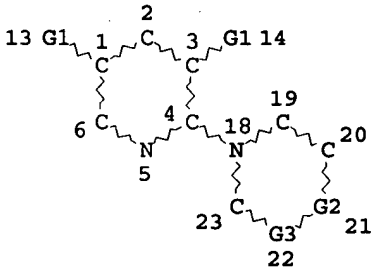
L19 STR



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VAR G2=C/N/O
REP G3=(0-2) C
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
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L26 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L21

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L26 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:758628 HCAPLUS
DOCUMENT NUMBER: 141:282402
TITLE: Hair dye composition comprising a heterocyclic oxidation base and a 2,3,5-triaminopyridine

coupler
INVENTOR(S): Kravtchenko, Sylvain; Lagrange, Alain; Vidal, Laurent; Fadli, Aziz
PATENT ASSIGNEE(S): L'Oreal, Fr.
SOURCE: Fr. Demande, 29 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2852241	A1	20040917	FR 2003-3115	20030313
EP 1459732	A1	20040922	EP 2004-290634	20040309

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

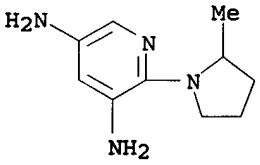
PRIORITY APPLN. INFO.: FR 2003-3115 A 20030313

OTHER SOURCE(S): MARPAT 141:282402

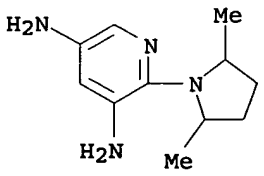
AB The title compns. are used for the dyeing of keratinous fibers. A hair dye composition contained 7-dimethylamino-3-aminopyrazolopyrimidine 2x10-3, 3,5-diamino-2-pyrrolidinopyridine 2x10-3, benzyl alc. 2, ethoxylated polyethylene glycol 3, ethanol 18, Oramix CG110 10, sodium metabisulfite 0.205, sequestering agent q.s., and water q.s. 100 g.

IT **756498-17-6**, N-(3,5-Diaminopyridin-2-yl)-2-methylpyrrolidine **756498-41-6 756498-45-0 756498-48-3 756498-50-7 756498-56-3 756498-59-6**
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(hair dye composition comprising heterocyclic oxidation base and 2,3,5-triaminopyridine coupler)

RN 756498-17-6 HCAPLUS
CN 3,5-Pyridinediamine, 2-(2-methyl-1-pyrrolidinyl)- (9CI) (CA INDEX NAME)

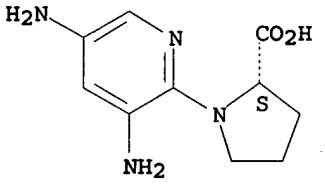


RN 756498-41-6 HCAPLUS
CN 3,5-Pyridinediamine, 2-(2,5-dimethyl-1-pyrrolidinyl)- (9CI) (CA INDEX NAME)

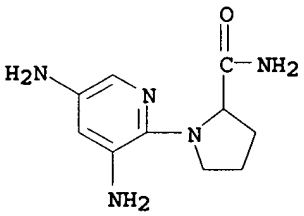


RN 756498-45-0 HCAPLUS
CN L-Proline, 1-(3,5-diamino-2-pyridinyl)- (9CI) (CA INDEX NAME)

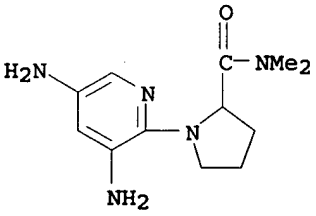
Absolute stereochemistry.



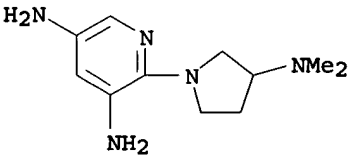
RN 756498-48-3 HCAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(3,5-diamino-2-pyridinyl)- (9CI) (CA INDEX NAME)



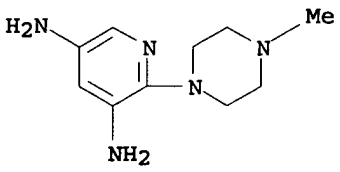
RN 756498-50-7 HCAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(3,5-diamino-2-pyridinyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 756498-56-3 HCAPLUS
CN 3,5-Pyridinediamine, 2-[3-(dimethylamino)-1-pyrrolidinyl]- (9CI) (CA INDEX NAME)



RN 756498-59-6 HCAPLUS
CN 3,5-Pyridinediamine, 2-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



IC ICM A61K007-13
CC 62-3 (Essential Oils and Cosmetics)
IT 51-35-4, 4-Hydroxyproline 109-01-3 110-85-0, Piperazine, biological studies 110-89-4, Piperidine, biological studies 111-49-9, Homopiperidine 123-75-1, Pyrrolidine, biological studies 147-85-3, Proline, biological studies 498-63-5, 2-Hydroxymethylpyrrolidine 504-03-0, 2,6-Dimethylpiperidine 535-75-1, 2-Carboxypiperidine 567-36-2, 3-Hydroxyproline 765-38-8, 2-Methylpyrrolidine 2812-47-7, 2-Pyrrolidinecarboxamide 3378-71-0, 2,5-Dimethylpyrrolidine 3433-37-2, 2-Hydroxymethylpiperidine 4318-37-0, N-Methyl homopiperazine 4606-65-9, 3-Hydroxymethylpiperidine 5227-53-2 5382-16-1, 4-Hydroxypiperidine 5626-66-4, 2,5-Pyrrolidinedimethanol 6859-99-0, 3-Hydroxypiperidine 19889-77-1, 2-Piperidinecarboxamide 27230-48-4, 3-Hydroxy-2-hydroxymethylpiperidine 40499-83-0, 3-Hydroxypyrrolidine 53427-65-9 67523-79-9D, derivs. 69478-75-7, 3-Dimethylaminopyrrolidine 79286-79-6, 3-Aminopyrrolidine 83030-08-4, 3-Methylaminopyrrolidine 89364-91-0, 3-Hydroxy-2-carboxamidopyrrolidine 99319-03-6, 2,4-Pyrrolidinedicarboxylic acid 128508-51-0 130497-29-9 169750-98-5 178105-25-4 188925-57-7 433980-61-1 473541-96-7, 3,4-Dihydroxypyrrolidine **756498-17-6**, N-(3,5-Diaminopyridin-2-yl)-2-methylpyrrolidine 756498-39-2, N-(3,5-Diaminopyridin-2-yl)pyrrolidine **756498-41-6** **756498-45-0** 756498-46-1 **756498-48-3** **756498-50-7** 756498-52-9 756498-54-1 **756498-56-3** 756498-58-5 **756498-59-6** 757967-87-6 757967-88-7 757967-89-8 757967-90-1 757967-91-2
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(hair dye composition comprising heterocyclic oxidation base and 2,3,5-triaminopyridine coupler)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:753132 HCAPLUS
DOCUMENT NUMBER: 141:265564
TITLE: Coupling agents having a 2,3,5-triaminopyridine structure and their use for dyeing keratinic fibers
INVENTOR(S): Fadli, Aziz; Vidal, Laurent
PATENT ASSIGNEE(S): L'oreal, Fr.
SOURCE: Eur. Pat. Appl., 36 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1457199	A1	20040915	EP 2004-290611	20040305
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
FR 2852240	A1	20040917	FR 2003-3114	20030313
JP 2004277423	A2	20041007	JP 2004-71608	20040312
US 2005081313	A1	20050421	US 2004-798454	20040312
PRIORITY APPLN. INFO.:			FR 2003-3114 A	20030313
			US 2003-467124P P	20030502

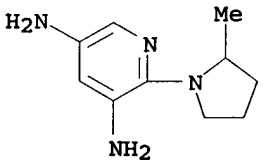
OTHER SOURCE(S): MARPAT 141:265564

AB Hair dye compns. comprising 2,3,5-triaminopyridine structure are used as coupling agent for dyeing hair. Thus, 2-(3,5-dimethylpiperidin-1-yl)pyridine-3,5-diamine (I) was prepared by the reduction of 2-(3,5-dimethylpiperidin-1 -yl)-3,5-dinitropyridine on palladium/charcoal. A hair dye composition contained I 10-3 mole, 2-[(4-Amino-phenyl)-(2-hydroxyethyl)-amino]-ethanol sulfate 10-3 mole, and water and excipients q.s. 100 g.

IT **756498-17-6 756498-41-6 756498-43-8 756498-45-0 756498-48-3 756498-50-7 756498-56-3 756498-59-6**
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(coupling agents having triaminopyridine structure and their use for dyeing keratinic fibers)

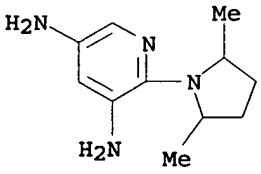
RN 756498-17-6 HCAPLUS

CN 3,5-Pyridinediamine, 2-(2-methyl-1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 756498-41-6 HCAPLUS

CN 3,5-Pyridinediamine, 2-(2,5-dimethyl-1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 756498-43-8 HCAPLUS
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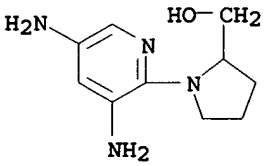
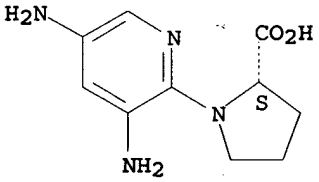
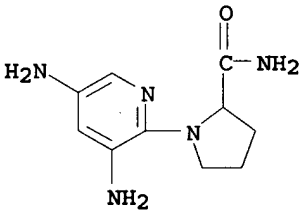


RN 756498-45-0 HCAPLUS
CN L-Proline, 1-(3,5-diamino-2-pyridinyl)- (9CI) (CA INDEX NAME)

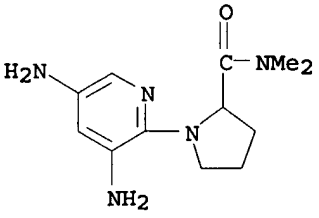
Absolute stereochemistry.



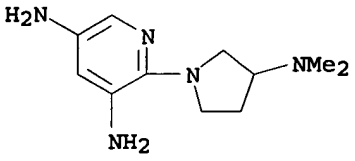
RN 756498-48-3 HCAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(3,5-diamino-2-pyridinyl)- (9CI) (CA INDEX NAME)



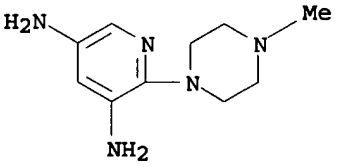
RN 756498-50-7 HCAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(3,5-diamino-2-pyridinyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 756498-56-3 HCAPLUS
CN 3,5-Pyridinediamine, 2-[3-(dimethylamino)-1-pyrrolidinyl]- (9CI) (CA INDEX NAME)



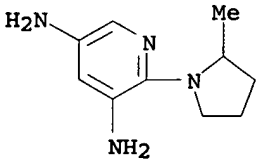
RN 756498-59-6 HCAPLUS
CN 3,5-Pyridinediamine, 2-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



IT **756498-18-7P 756498-20-1P 756498-23-4P**
756498-25-6P 756498-27-8P 756498-29-0P
756498-31-4P 756498-33-6P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(coupling agents having triaminopyridine structure and their use for dyeing keratinic fibers)
RN 756498-18-7 HCAPLUS
CN Methanol, compd. with 2-(2-methyl-1-pyrrolidinyl)-3,5-pyridinediamine hydrochloride (5:5:9) (9CI) (CA INDEX NAME)

CM 1

CRN 756498-17-6
CMF C10 H16 N4

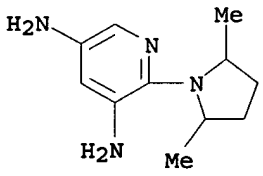


CM 2

CRN 67-56-1
CMF C H4 O

H_3C-OH

RN 756498-20-1 HCAPLUS
CN 3,5-Pyridinediamine, 2-(2,5-dimethyl-1-pyrrolidinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 756498-23-4 HCAPLUS
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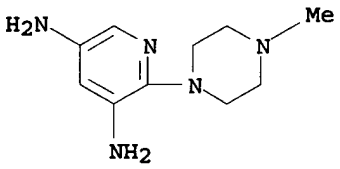

●2 HCl

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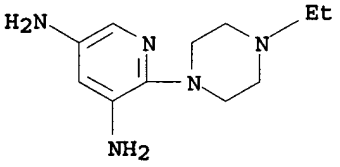
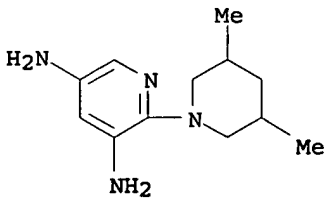
CN 3,5-Pyridinediamine, 2-(4-ethyl-1-piperazinyl)-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

RN 756498-27-8 HCAPLUS
CN 3,5-Pyridinediamine, 2-(3,5-dimethyl-1-piperidinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 756498-29-0 HCAPLUS
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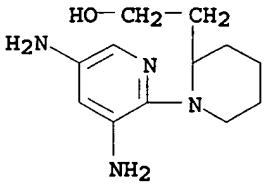
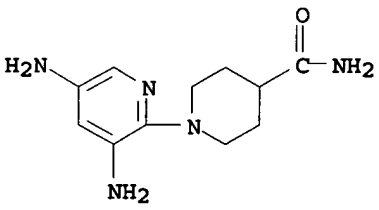


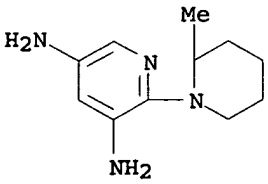
●2 HCl

RN 756498-31-4 HCAPLUS
CN 4-Piperidinecarboxamide, 1-(3,5-diamino-2-pyridinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

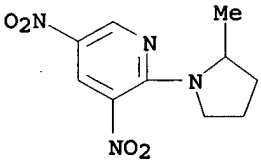
RN 756498-33-6 HCAPLUS
CN 3,5-Pyridinediamine, 2-(2-methyl-1-piperidinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



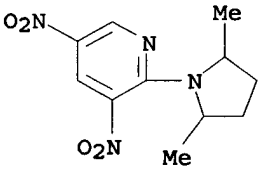
●2 HCl

IT **756498-19-8P 756498-21-2P 756498-24-5P**
756498-26-7P 756498-28-9P 756498-30-3P
756498-32-5P 756498-34-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(coupling agents having triaminopyridine structure and their use for dyeing keratinic fibers)

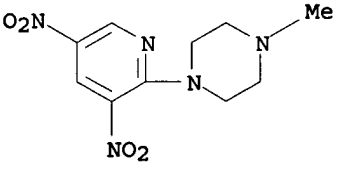
RN 756498-19-8 HCAPLUS
CN Pyridine, 2-(2-methyl-1-pyrrolidinyl)-3,5-dinitro- (9CI) (CA INDEX NAME)



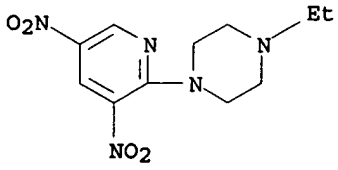
RN 756498-21-2 HCAPLUS
CN Pyridine, 2-(2,5-dimethyl-1-pyrrolidinyl)-3,5-dinitro- (9CI) (CA INDEX NAME)



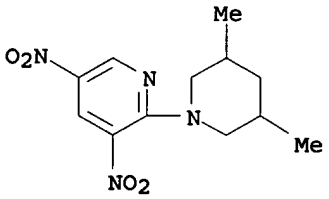
RN 756498-24-5 HCAPLUS
CN Piperazine, 1-(3,5-dinitro-2-pyridinyl)-4-methyl- (9CI) (CA INDEX NAME)



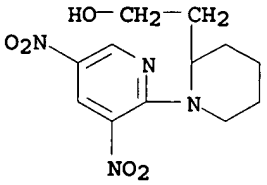
RN 756498-26-7 HCAPLUS
CN Piperazine, 1-(3,5-dinitro-2-pyridinyl)-4-ethyl- (9CI) (CA INDEX NAME)



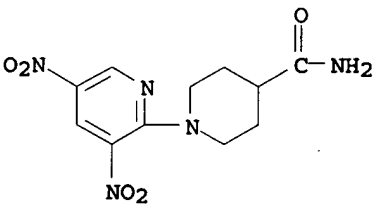
RN 756498-28-9 HCAPLUS
CN Pyridine, 2-(3,5-dimethyl-1-piperidinyl)-3,5-dinitro- (9CI) (CA INDEX NAME)



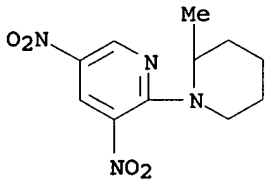
RN 756498-30-3 HCAPLUS
CN 2-Piperidineethanol, 1-(3,5-dinitro-2-pyridinyl)- (9CI) (CA INDEX NAME)



RN 756498-32-5 HCAPLUS
CN 4-Piperidinecarboxamide, 1-(3,5-dinitro-2-pyridinyl)- (9CI) (CA INDEX NAME)



RN 756498-34-7 HCAPLUS
CN Pyridine, 2-(2-methyl-1-piperidinyl)-3,5-dinitro- (9CI) (CA INDEX NAME)



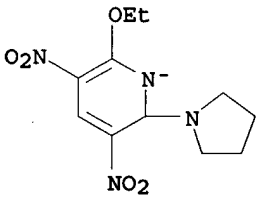
IC ICM A61K007-13
ICS C07D401-04; C07D413-04
CC 62-3 (Essential Oils and Cosmetics)
IT **756498-17-6** 756498-39-2 **756498-41-6**
756498-43-8 **756498-45-0** 756498-46-1
756498-48-3 **756498-50-7** 756498-52-9
756498-54-1 **756498-56-3** 756498-58-5
756498-59-6
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(coupling agents having triaminopyridine structure and their use for dyeing keratinic fibers)
IT 756498-14-3P 756498-15-4P **756498-18-7P**
756498-20-1P 756498-22-3P **756498-23-4P**
756498-25-6P **756498-27-8P** **756498-29-0P**
756498-31-4P **756498-33-6P** 756498-36-9P
756498-38-1P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(coupling agents having triaminopyridine structure and their use for dyeing keratinic fibers)
IT 90871-11-7P 134787-63-6P 573987-10-7P 756498-16-5P
756498-19-8P **756498-21-2P** **756498-24-5P**
756498-26-7P **756498-28-9P** **756498-30-3P**
756498-32-5P **756498-34-7P** 756498-37-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(coupling agents having triaminopyridine structure and their use for dyeing keratinic fibers)
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:354713 HCAPLUS
DOCUMENT NUMBER: 139:164474
TITLE: Kinetic and equilibrium studies of σ-adduct formation and nucleophilic substitution in the reactions of 2-phenoxy-3,5-dinitropyridine and 2-ethoxy-3,5-dinitropyridine with aliphatic amines in dipolar aprotic solvents
AUTHOR(S): Crampton, Michael R.; Emokpae, Thomas A.; Howard, Judith A. K.; Isanbor, Chukwuemeka; Mondal, Raju
CORPORATE SOURCE: Chemistry Department, Durham University, Durham, DH1 3LE, UK
SOURCE: Organic & Biomolecular Chemistry (2003), 1(6), 1004-1011
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:164474
AB The reactions of aliphatic amines with 2-phenoxy-3,5-dinitropyridine, 4, and 2-ethoxy-3,5-dinitropyridine, 5, in DMSO result in the rapid reversible formation of anionic σ-adducts at the

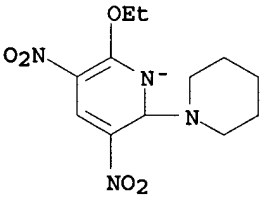
6-position. Kinetic studies show that proton transfer from the initially formed zwitterions to base may be rate-limiting. Slower reactions result, except in the case of 5 and piperidine, in displacement of the 2-substituent via intermediates which have lower thermodn. stabilities than their 6-isomers. Base catalysis of the substitution process is attributed in the case of 4 to rate-limiting proton transfer from zwitterionic intermediates, but in 5 to acid catalysis of ethoxide departure (SB-GA mechanism). X-ray crystallog. of 5 shows a planar nonstrained structure although the structure of 2-piperidino-3,5-dinitropyridine, 10c, shows distortion resulting from steric interactions of the 2- and 3-substituents. Kinetic and equilibrium results are compared with those for related reactions of the more sterically strained 2,4,6-trinitrobenzene derivs. Results for the reactions of 4 and 5 with pyrrolidine in three dipolar aprotic solvents are compared. Values of equilibrium consts. for σ-adduct formation decrease in the order DMSO > DMF >> acetonitrile, while values of rate consts. for proton transfer are in the reverse order.

IT **573987-11-8 573987-12-9**
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(kinetics and equilibrium of σ-adduct formation and nucleophilic substitution in reactions of 2-phenoxy- and 2-ethoxy-3,5-dinitropyridine with aliphatic amines in dipolar aprotic solvents)

RN 573987-11-8 HCAPLUS
CN Pyridine, 6-ethoxy-1,2-dihydro-3,5-dinitro-2-(1-pyrrolidinyl)-, ion(1-) (9CI) (CA INDEX NAME)



RN 573987-12-9 HCAPLUS
CN Pyridine, 6-ethoxy-1,2-dihydro-3,5-dinitro-2-(1-piperidinyl)-, ion(1-) (9CI) (CA INDEX NAME)



CC 22-12 (Physical Organic Chemistry)
Section cross-reference(s): 75

IT **573987-11-8 573987-12-9**
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(kinetics and equilibrium of σ-adduct formation and nucleophilic substitution in reactions of 2-phenoxy- and

2-ethoxy-3,5-dinitropyridine with aliphatic amines in dipolar aprotic solvents)
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:608919 HCAPLUS
DOCUMENT NUMBER: 105:208919
TITLE: Quinazoline derivatives and antihypertensive preparations containing them
INVENTOR(S): Yokoyama, Keiichi; Kato, Koji; Kitahara, Takumi; Ohno, Hiroyasu; Nishina, Takashi; Awaya, Akira; Nakano, Takuo; Watanabe, Kazuyuki; Saruta, Sakae; Kumakura, Mikio
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan; Mitsui Pharmaceuticals, Inc.
SOURCE: Eur. Pat. Appl., 235 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 188094	A2	19860723	EP 1985-309049	1985 1212
EP 188094	A3	19871223		
EP 188094	B1	19920318		
R: DE, FR, GB, IT				
JP 61140568	A2	19860627	JP 1984-263015	1984 1214
JP 05028709	B4	19930427		
JP 62056488	A2	19870312	JP 1985-194968	1985 0905
JP 03071430	B4	19911113		
JP 62067077	A2	19870326	JP 1985-204463	1985 0918
JP 05029223	B4	19930428		

PRIORITY APPLN. INFO.:
JP 1984-263015 A 1984 1214
JP 1985-194968 A 1985 0905
JP 1985-204463 A 1985 0918

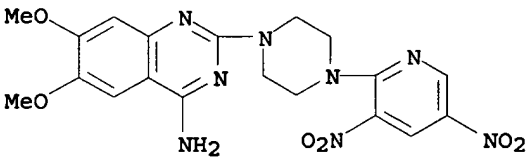
OTHER SOURCE(S): CASREACT 105:208919; MARPAT 105:208919
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

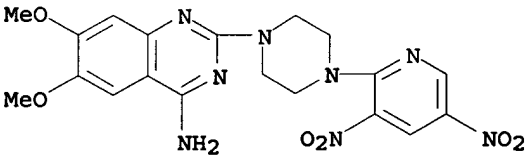
AB Piperazinyl- and homopiperazinylquinazolines I (R1 = H, MeO; R2, R3 = H, alkoxy; R4 = H, NH2; R5 = substituted 2-pyrimidinyl, 2-pyridinyl, 2-quinolinyl, fused pyrimidinyl; n = 2, 3) were prepared as antihypertensives. Thus, 4-benzyl-1-piperazinecarboxamidine sulfate was cyclocondensed with MeCOC(CO2Me):CHOMe to give pyrimidinecarboxylate II. This was amidated with EtNH2 and cyclocondensed with DMF to give pyridopyrimidinone III, which was debenzylated and condensed with 4-amino-2-chloro-6,7-dimethoxyquinazoline to give piperazinylquinazoline IV. In rats 1 mg IV/kg orally reduced blood pressure 23.0% after 6 h, the effect lasting 24 h. Tablets were prepared each containing I 1, starch 60, microcrystn. cellulose 35, light silica 3, and Mg stearate 1 mg.

IT **104965-86-8P 104987-66-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antihypertensive)

RN 104965-86-8 HCAPLUS
CN 4-Quinazolinamine, 2-[4-(3,5-dinitro-2-pyridinyl)-1-piperazinyl]-6,7-dimethoxy- (9CI) (CA INDEX NAME)



RN 104987-66-8 HCAPLUS
CN 4-Quinazolinamine, 2-[4-(3,5-dinitro-2-pyridinyl)-1-piperazinyl]-6,7-dimethoxy-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

IC ICM C07D471-04
ICS C07D487-04; C07D239-84; C07D495-04; C07D401-12; A61K031-495; A61K031-505

ICI C07D471-04, C07D239-00, C07D221-00; C07D487-04, C07D239-00, C07D209-00; C07D487-04, C07D243-00, C07D239-00; C07D495-04, C07D333-00, C07D239-00; C07D487-04

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT 102839-00-9P 104964-10-5P 104964-11-6P 104964-12-7P
104964-13-8P 104964-14-9P 104964-15-0P 104964-16-1P
104964-17-2P 104964-18-3P 104964-19-4P 104964-20-7P
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104964-25-2P 104964-26-3P 104964-27-4P 104964-28-5P
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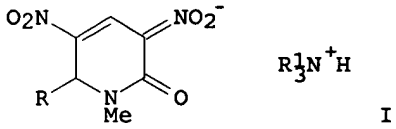
104987-66-8P 105010-30-8P 105201-43-2P 105201-44-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antihypertensive)

L26 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:488003 HCAPLUS
DOCUMENT NUMBER: 99:88003
TITLE: Nucleophilic reaction upon electron-deficient pyridone derivatives. V. Anionic σ-adducts of 1-methyl-3,5-dinitro-2-pyridone
AUTHOR(S): Tohda, Yasuo; Ariga, Masahiro; Kawashima, Toshihide; Matsumura, Eizo
CORPORATE SOURCE: Dep. Chem., Osaka Kyoiku Univ., Osaka, 543, Japan
SOURCE: Chemistry Letters (1983), (5), 715-18
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Alkylammonium salts I of anionic σ-adducts of 1-methyl-3,5-dinitro-2-pyridone with amine and C nucleophiles were isolated and characterized. The C adducts are more stable than the amine adducts, which dissociate in dilute MeOH. The acetone adduct was converted into 4-nitro-1-pyrrolidinylbenzene quant. by heating with pyrrolidine.

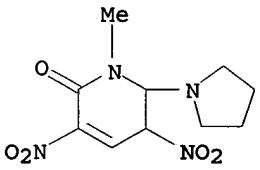
IT **86670-27-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 86670-27-1 HCAPLUS

CN 2(1H)-Pyridinone, 5,6-dihydro-1-methyl-3,5-dinitro-6-(1-pyrrolidinyl)-, compd. with pyrrolidine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 86670-26-0
CMF C10 H14 N4 O5



CM 2

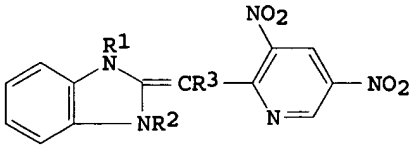
CRN 123-75-1
CMF C4 H9 N

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

IT 10220-22-1P 86653-20-5P 86653-22-7P 86653-24-9P
86653-26-1P 86653-32-9P 86653-35-2P 86653-37-4P
86653-39-6P **86670-27-1P** 86714-58-1P 86714-59-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L26 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:203958 HCAPLUS
DOCUMENT NUMBER: 90:203958
TITLE: Products of the reaction of benzimidazole derivatives with 2-chloro-3,5-dinitropyridine
AUTHOR(S): Zakhs, E. R.; Subbotina, M. A.; El'tsov, A. V.
CORPORATE SOURCE: USSR
SOURCE: Zhurnal Organicheskoi Khimii (1979), 15(1),

200-6
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 90:203958
GI



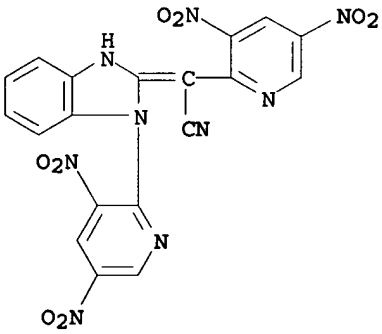
I

AB Benzimidazoles I (R1 = 3,5-dinitro-2-pyridyl, Me; R2 = H, Me; R3 = CN, H, CO2Me) were prepared in 50-90% yields by treating benzimidazoleacetonitriles with 2-chloro-3,5-dinitropyridine, follows by methylation, hydration, esterification, or protonation (to give the endocyclic onium compds.).

IT **70309-18-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and isomerism of)

RN 70309-18-1 HCAPLUS

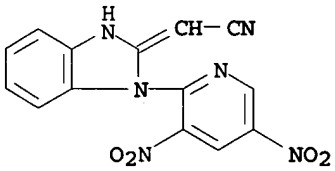
CN 2-Pyridineacetonitrile, α-[1-(3,5-dinitro-2-pyridinyl)-1,3-dihydro-2H-benzimidazol-2-ylidene]-3,5-dinitro- (9CI) (CA INDEX NAME)



IT **70309-19-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and protonation of)

RN 70309-19-2 HCAPLUS

CN Acetonitrile, [1-(3,5-dinitro-2-pyridinyl)-1,3-dihydro-2H-benzimidazol-2-ylidene]- (9CI) (CA INDEX NAME)



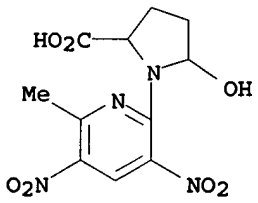
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))

IT **70309-18-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and isomerism of)
IT **70309-19-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and protonation of)

L26 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1970:78819 HCAPLUS
DOCUMENT NUMBER: 72:78819
TITLE: Synthesis and properties of 2-fluoro-3,5-dinitro-4-methyl-pyridine and 2-fluoro-3,5-dinitro-6-methylpyridine
AUTHOR(S): Talik, Tadeusz; Talik, Zofia
CORPORATE SOURCE: Wyzsza Szk. Ekon., Wroclaw, Pol.
SOURCE: Roczniki Chemii (1969), 43(11), 1961-70
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: German
AB The title compds. were synthesized via the following products: 2-nitramino-5-nitro-4-picoline (I), 2-amino-3,5-dinitro-4-picoline (II), 2-fluoro-3,5-dinitro-4-picoline (III); and 2-nitramino-5-nitro-6-picoline (IV), 2-amino-3,5-dinitro-6-picoline (V) and 2-fluoro-3,5-dinitro-6-picoline (VI). The fluorine atom in III and VI was easily substituted in reactions with H+-H2O, alcs., amines, and amino acids. Thus, 10 g I or IV (optionally containing some of the 3-NO2 isomer)in 50 ml concentrated H2SO4 was heated 1 hr on a steam bath to give 7.1 g II, m. 183°, or 7.7 g V, m. 179°, (both from EtOH-Me2NCHO), resp. II or V (6.0 g) was dissolved in a solution of HBF4 (from 30 g H3BO3 and 75 ml 38% HF aqueous), 9 g NaNO2 slowly added at 0°, and the mixture kept 20 min at room temperature to yield 2.7 g III, m. 33°, or 2.5 g VI, b3 122-3°, m. 35°, resp. III or VI was refluxed in 5 ml 1:1 HCl-H2O 10 min to give 95.2% 2-hydroxy-3,5-dinitro-4-picoline, m. 254° (decomposition) (H2O-Me2NCHO), or 98.5% 2-hydroxy-3,5-dinitro-6-picoline m. 238° (decomposition),(H2O-EtOH), resp. III or VI (0.5 g) was refluxed with 5 ml MeOH or EtOH 90min to give 94.6% 2-methoxy-3,5-dinitro-4-picoline, m. 129°; 95.5% 2-ethoxy-3,5-dinitro-4-picoline, m. 87°; 94.4% 2-methoxy-3,5-dinitro-6-picoline, m. 54°; and 2-ethoxy-3,5-dinitro-6-picoline, m. 63°, resp. (all recrystd. from aqueous EtOH). To 0.5 g II in 3 ml EtOH was added 3 ml saturated NH3, or gaseousamine solution in EtOH, or 3 ml liquid amine to give R- in 2-(R-substituted)-3,5-dinitro-4-picolines (VII) (R, % yield, and m.p. given): NH2, 98.5, 187° (H2O-Me2-HCHO); NHEt, 99.2, 103° (H2O-EtOH); NHCH2CH2OH, 95.9, 118° (H2O-EtOH); NHPh, 88.2, 156° (C6H6-EtOH); NHNHPh, 95.4, 126° (decomposition) (EtOH); NMe2, 88.9, 74° (EtOH); and NEt2, 94.9, 87° (H2O-EtOH). From VI by the above procedure were obtained 2-(R-substituted)-3,5-dinitro-6-picolines (VIII) (same data given): NH2, 99.1, 179°(EtOH-H2O); NHEt, 89.3, 80° (EtOH-H2O); NHCH2CH2OH, 98.4, 105° (EtOH-H2O); NHPh, 95.1, 163° (C6H6-EtOH); NHNHPh, 95.5, 150° (EtOH-Me2NCHO); NMe2, 95.4, 84° (EtOH); and NEt2, 82.1, 52° (EtOH-H2O). III (0.005 mole) in 10 ml EtOH was added to a solution of an amino acid (0.005 mole in 5 ml H2O and 0.01 mole NaHCO3), and the mixture kept 10 min at room temperature to give the following VII (same data given): NHCHMeCO2H-DL, 80.2, 166° (H2O-EtOH); NHCH(CH2OH)CO2H-DL, 77.5, 160° (decomposition) (H2O-EtOH); NHCH(CH2CH2SMe)CO2H-L, 92.4, 163° (decomposition) (EtOH-Me2NCHO); and NHCH(CH2CO2H)CO2-H-L, 90.5, 162° (decomposition) (H2O-EtOH). Similarly VI gave the following VIII (same data given): NHCH2CO2H, 95.5, 209° (decomposition) (H2O-Me2NCHO); NHCHMeCO2H-DL, 82.1, 121° (EtOH-H2O); NHCH(CH2CONH2)CO2H-L, 78.5, 180° (H2O-EtOH); and

N-(L-hydroxyprolinyl), 78.5, 55° (H2O-EtOH).
IT **25864-44-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 25864-44-2 HCAPLUS
CN Proline, 5-hydroxy-1-(6-methyl-3,5-dinitro-2-pyridyl)- (8CI) (CA INDEX NAME)



CC 27 (Heterocyclic Compounds (One Hetero Atom))
IT 25782-38-1P 25782-39-2P 25782-40-5P 25782-41-6P
25782-42-7P 25782-43-8P 25782-44-9P 25782-45-0P
25782-46-1P 25864-29-3P 25864-30-6P 25864-31-7P
25864-32-8P 25864-33-9P 25864-34-0P 25864-35-1P
25864-36-2P 25864-37-3P 25864-38-4P 25864-39-5P
25864-40-8P 25864-41-9P 25864-42-0P 25864-43-1P
25864-44-2P 25979-16-2P 25979-17-3P 26169-30-2P
30505-22-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L26 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1969:47456 HCAPLUS
DOCUMENT NUMBER: 70:47456
TITLE: 4-Nitroimidazoles
INVENTOR(S): Klink, Rainer; Hepding, Ludwig
PATENT ASSIGNEE(S): Merck, E., A.-G.
SOURCE: Brit., 5 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1133408		19681113	GB 1967-38544	1967 0822
DE 1620043			DE	
DE 1695397			DE	
FR 7260			FR	
US 3491105		19700120	US	1967 0925
ZA 6905397		19690000	ZA	
PRIORITY APPLN. INFO.:			DE	1966 1015
			DE	1967 0301

OTHER SOURCE(S): MARPAT 70:47456

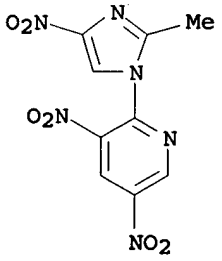
GI For diagram(s), see printed CA Issue.

AB The title compds. of formula I with antitrichomonadal activity, are prepared by alkylation of 2-substituted-4(5)-nitroimidazoles. Thus, a mixture of 2.3 g. Na in 100 ml. EtOH, 11.3 g. 4(5)-nitroimidazole, and 17 g. 2-chloro-5-nitropyridine was refluxed 15 min. and poured into H2O to give 19 g. I (R1 = H, R2 = 5-nitro-2-pyridyl), m. 196-8° (Me2CO-petroleum ether). Heating a mixture of 15 g. 2-methyl-4(5)-nitroimidazole Na salt (II), 15.7 g. p-O2NC6H4Cl, and 100 ml. PrOH in a sealed tube 30 min. at 150° gave 18.5 g. I (R1 = Me, R2 = p-O2NC6H4)(III). Similarly, refluxing a mixture of 15 g. II, 14.1 g. p-O2NC6H4F (IV), and 100 ml. Me2NCHO 15 min. gave 15 g. III, m. 185-7° (Me2CO). The following I were similarly prepared (R1, R2, and m.p. given): H, 3-nitro-2-pyridyl, 144-6°; H, 3,5-dinitro-2-pyridyl, 146-9°; H, p-O2NC6H4, 188-90°; H, o-O2NC6H4, 123-5°; Me, o-O2NC6H4, 177-9°; H, 2,4-(O2N)2C6H3, 154-6°; Me, 2,4-(O2N)2C6H3, 194-6°; H, 2,4-Me-(O2N)C6H3, 185-7°; Me, 2,4-Me(O2N)C6H3, 196-7°; Me, 3,4-Me(O2N)C6H3, 176-8°; Me, 5-nitro-2-pyridyl, 175-8°; Me, 3-nitro-2-pyridyl, 179-82°; and Me, 3,5-dinitro-2-pyridyl, 150-2°. Heating a mixture of 101.5 g. 1-(4-nitrophenyl)-2-methylimidazole (V) (m. 134-5°)(obtained by stirring 2-methylimidazole and IV 2 hrs. at 120-5° in Me2NCHO), 200 ml. 65% aqueous HNO3, and 50 ml. concentrated H2SO4 1 hr. at 120° with portionwise addition of 150 ml. concentrated H2SO4 and working up gave 5.1 g. III and 16 g. 1-(4-nitrophenyl)-2-methyl-5-nitroimidazole, m. 164.5-5.5°; 19.5 g. V was recovered.

IT **21722-03-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21722-03-2 HCAPLUS

CN Pyridine, 2-(2-methyl-4-nitroimidazol-1-yl)-3,5-dinitro- (8CI) (CA INDEX NAME)



IC C07D

CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 21721-89-1P 21721-90-4P 21721-91-5P 21721-92-6P
21721-93-7P 21721-94-8P 21721-95-9P 21721-96-0P
21721-97-1P 21721-98-2P 21721-99-3P 21722-00-9P
21722-01-0P 21722-02-1P **21722-03-2P** 21722-04-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L26 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1965:480971 HCAPLUS

DOCUMENT NUMBER: 63:80971

ORIGINAL REFERENCE NO.: 63:14976f-g

TITLE: The intramolecular participation of the pyridyl group in the acid hydrolysis of dinitropyridyl dipeptides

AUTHOR(S): Signor, Angelo; Bordignon, Emilio

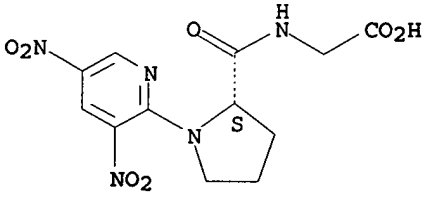
CORPORATE SOURCE: Univ. Padua, Italy

SOURCE: Journal of Organic Chemistry (1965), 30(10), 3447-51
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Measurements are reported on the kinetics of hydrolysis of dinitro-2-pyridylalanylglycine in solutions of hydrochloric acid up to 10M; acid-catalyzed hydrolysis of the amide bond occurs when the acid concentration is 2M or higher and the rate of hydrolysis is accurately proportional to H0; classification of the reaction according to Bunnett gives an ω value of zero and this indicates that water does not participate in transformation of SH+ to a transition state. Furthermore the kinetic results for other dinitro-2-pyridyl dipeptides show that the catalytic effect is a general phenomenon. On the other hand, the hydrolysis of dinitro-2-pyridylalanylgiycine is about 102-103 times as fast as the hydrolyses of dinitrophenylalanylglycine and of dinitro4-pyridylalanylglycine. These results suggest that the acid-catalyzed hydrolysis of dinitro-2-pyridyl dipeptides is an electrophilic-nucleophilic catalyzed reaction involving a cyclic aeylpyridinium intermediate.

IT **2900-30-3**, Glycine, N-[1-(3,5-dinitro-2-pyridyl)prolyl]- (hydrolysis of)
RN 2900-30-3 HCAPLUS
CN Glycine, N-[1-(3,5-dinitro-2-pyridyl)-L-prolyl]- (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 44 (Amino Acids, Peptides, and Proteins)
IT 2900-13-2, Alanine, N-[N-(3,5-dinitro-2-pyridyl)alanyl]-
2900-29-0, Alanine, N-[N-(3,5-dinitro-2-pyridyl)glycyl]-
2900-30-3, Glycine, N-[1-(3,5-dinitro-2-pyridyl)prolyl]-
2900-31-4, Serine, N-[N-(3,5-dinitro-2-pyridyl)glycyl]-
2900-32-5, Leucine, N-[N-(3,5-dinitro-2-pyridyl)leucyl]-
2900-33-6, Alanine, N-[N-(3,5-dinitro-2-pyridyl)alanyl]-3-phenyl-
2900-34-7, Glycine, N-[N-(3,5-dinitro-2-pyridyl)alanyl]-
2900-35-8, Glycine, N-[N-(2,4-dinitrophenyl)alanyl]- 2900-36-9, Glycine, N-[N-(3,5-dinitro-2-pyridyl)glycyl]- (hydrolysis of)

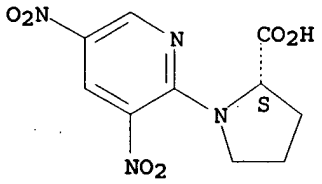
L26 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1965:86288 HCAPLUS
DOCUMENT NUMBER: 62:86288
ORIGINAL REFERENCE NO.: 62:15402g-h
TITLE: Thin-layer chromatography of dinitropyridyl- and nitropyrimidylamino acids
AUTHOR(S): Di Bello, Carlo; Signor, Angelo
CORPORATE SOURCE: Univ. Padua, Italy
SOURCE: Journal of Chromatography (1965), 17(3), 506-12
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB One to 2 γ of sample was spotted on silica gel G coated plates. When the solvent front had travelled 10 cm., the plates

were removed and the solvent evaporated under a current of hot air. For 2-dimensional chromatog. the sample was applied onto the diagonal of the plate. For maximum reproducibility the plates must be dried between dimension runs at constant conditions. Spraying with 1% KMnO4 followed by N HCl revealed nitropyrimidylamino acids as yellow spots on a pink background; they next appeared as black spots when sprayed with 8.1% HgNO3 in 0.5N HNO3, then 0.5N HNO3, then, after drying, aqueous (NH4)2S. Of 6 solvent systems tested, either in single or 2-dimensional chromatog., CHCl3-MeOH-AcOH (95:5:1) followed by PrOH-33% NH4OH (70:30) gave the best separation

IT **3264-09-3**, Proline, 1-(3,5-dinitro-2-pyridyl)-, L-
(chromatog. of)
RN 3264-09-3 HCAPLUS
CN Proline, 1-(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 2 (Analytical Chemistry)
IT 2980-33-8, 2-Pyridinol, 3,5-dinitro- 3073-24-3, Glutamic acid, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-25-4, Isoleucine, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-26-5, Leucine, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-27-6, Serine, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-28-7, Threonine, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-29-8, Valine, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-30-1, Pyridine, 2-amino-3,5-dinitro- 3073-32-3, Aspartic acid, N-(5-nitro-2-pyrimidinyl)-, L- 3073-33-4, Glutamic acid, N-(5-nitro-2-pyrimidinyl)-, DL- 3073-34-5, Alanine, N-(5-nitro-2-pyrimidinyl)-, DL- 3073-68-5, Alanine, N-(5-nitro-2-pyrimidinyl)-3-phenyl-, DL- 3073-69-6, Glycine, N-(5-nitro-2-pyrimidinyl)-, L- 3073-70-9, Isoleucine, N-(5-nitro-2-pyrimidinyl)-, DL- 3073-71-0, Leucine, N-(5-nitro-2-pyrimidinyl)-, DL- 3073-72-1, Lysine, N2,N6-bis(5-nitro-2-pyrimidinyl)-, L- 3073-73-2, Serine, N-(5-nitro-2-pyrimidinyl)-, DL- 3073-74-3, Proline, 1-(5-nitro-2-pyrimidinyl)-, L- 3073-75-4, Threonine, N-(5-nitro-2-pyrimidinyl)-, DL- 3073-76-5, Valine, N-(5-nitro-2-pyrimidinyl)-, DL- 3073-77-6, Pyrimidine, 2-amino-5-nitro- 3264-06-0, Alanine, N-(3,5-dinitro-2-pyridyl)-, DL- 3264-07-1, Alanine, N-(3,5-dinitro-2-pyridyl)-3-phenyl-, DL- 3264-08-2, Glycine, N-(3,5-dinitro-2-pyridyl)- **3264-09-3**, Proline, 1-(3,5-dinitro-2-pyridyl)-, L- 3264-10-6, 2-Pyrimidinol, 5-nitro- 3426-97-9, Lysine, N2,N6-bis(3,5-dinitro-2-pyridyl)-, L- 3521-73-1, Aspartic acid, N-(3,5-dinitro-2-pyridyl)-, L
(chromatog. of)

L26 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1965:86287 HCAPLUS
DOCUMENT NUMBER: 62:86287
ORIGINAL REFERENCE NO.: 62:15402f-g
TITLE: Chromatographic separation of diketones. III. Chromatography of derivatives of 2-phenyl-1,3-indandione
AUTHOR(S): Kreicberga, D.; Gudriniece, E.
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1964), (4), 424-8

CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian

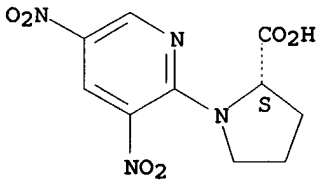
AB Derivs. (Cl, Br, I, NO2, NH2, Me2N Et2N, AcNH, MeO, SH, Me3N, MeEt2N) substituted in positions 2, 3, and 4 in the phenyl radical and in the 4 and 5 positions in the phthaloyl radical were tried. Best sepns. were achieved on powdered silica gel. Extensive tables, giving Rf values for 39 compds. in 12 different combinations of solvents and adsorbents are given.

IT **3264-09-3**, Proline, 1-(3,5-dinitro-2-pyridyl)-, L- (chromatography of)

RN 3264-09-3 HCAPLUS

CN Proline, 1-(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



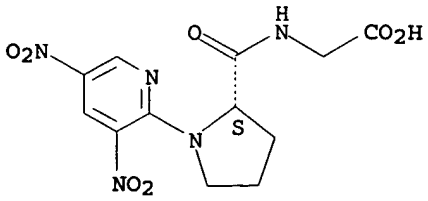
CC 2 (Analytical Chemistry)

IT 83-12-5, 1,3-Indandione, 2-phenyl 117-37-3, 1,3-Indandione, 2-(p-methoxyphenyl)- 606-23-5, 1,3-Indandione 969-63-1, 1,3-Indandione, 2-[p-(diethylamino)phenyl]- 1146-98-1, 1,3-Indandione, 2-(p-bromophenyl)- 1146-99-2, 1,3-Indandione, 2-(p-chlorophenyl)- 1147-00-8, 1,3-Indandione, 2-(p-iodophenyl)- 1153-90-8, 1,3-Indandione, 2-(p-nitrophenyl)- 1156-76-9, Acetanilide, 4'-(1,3-dioxo-2-indanyl)- 1225-30-5, 1,3-Indandione, 2-[p-(dimethylamino)phenyl]- 1470-34-4, 1,3-Indandione, 4-nitro-2-phenyl- 1470-35-5, 1,3-Indandione, 5-bromo-2-phenyl- 1470-36-6, 1,3-Indandione, 5-chloro-2-phenyl- 1470-37-7, 1,3-Indandione, 4-bromo-2-phenyl- 1470-38-8, 1,3-Indandione, 2-(3,4-dimethoxyphenyl)- 1470-39-9, 1,3-Indandione, 2-(o-methoxyphenyl)- 1470-40-2, 1,3-Indandione, 2-(o-iodophenyl)- 1470-41-3, 1,3-Indandione, 2-(o-bromophenyl)- 1470-42-4, 1,3-Indandione, 2-(o-chlorophenyl)- 1470-43-5, 1,3-Indandione, 2-(m-bromophenyl)- 1470-44-6, 1,3-Indandione, 2-(m-chlorophenyl)- 1470-52-6, 1,3-Indandione, 2-(p-(dimethylamino)phenyl]-4,5-dimethoxy- 1470-53-7, 1,3-Indandione, 4,5-dimethoxy-2-phenyl- 1470-54-8, 1,3-Indandione, 4-nitro-2-(p-nitrophenyl)- 1470-56-0, 1,3-Indandione, 4,5,6,7-tetrachloro-2-phenyl- 1640-36-4, 1,3-Indandione, 4-chloro-2-phenyl- 1640-37-5, 1,3-Indandione, 2-(m-iodophenyl)- 1641-12-9, 1,3-Indandione, 2-(3,4-dimethoxyphenyl)-4,5-dimethoxy- 1641-13-0, 1,3-Indandione, 4,5-dimethoxy-2-(p-methoxyphenyl)- 1641-14-1, 1,3-Indandione, 5-nitro-2-(p-nitrophenyl)- 1668-36-6, 1,3-Indandione, 2-(p-mercaptophenyl)- 1989-66-8, 1,3-Indandione, 4-iodo-2-phenyl- 2048-60-4, 1,3-Indandione, 5-iodo-2-phenyl- 2535-52-6, 1,3-Indandione, 5-nitro-2-phenyl- 2863-22-1, Acetanilide, 4'-(5-nitro-1,3-dioxo-2-indanyl)- 2878-47-9, Acetanilide, 4'-(4-nitro-1,3-dioxo-2-indanyl)- 2980-33-8, 2-Pyridinol, 3,5-dinitro- 3073-30-1, Pyridine, 2-amino-3,5-dinitro- 3073-68-5, Alanine, N-(5-nitro-2-pyrimidinyl)-3-phenyl-, DL- 3073-72-1, Lysine, N2,N6-bis(5-nitro-2-pyrimidinyl)-, L- 3073-74-3, Proline, 1-(5-nitro-2-pyrimidinyl)-, L- 3073-77-6, Pyrimidine, 2-amino-5-nitro- 3264-07-1, Alanine, N-(3,5-dinitro-2-pyridyl)-3-phenyl-, DL- **3264-09-3**, Proline, 1-(3,5-dinitro-2-pyridyl)-, L- 3264-10-6, 2-Pyrimidinol, 5-nitro- 3426-97-9, Lysine, N2,N6-bis(3,5-dinitro-2-pyridyl)-, L- 3457-74-7,

1,3-Indandione, 4,5,6,7-tetrahydro-2-phenyl- 92497-72-8,
1,3-Indandione, 4-(p-aminophenyl)-
(chromatography of)

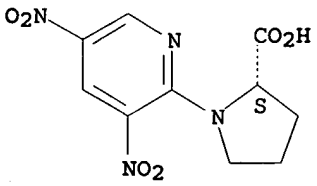
L26 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1964:485898 HCAPLUS
DOCUMENT NUMBER: 61:85898
ORIGINAL REFERENCE NO.: 61:15018h,15019a-d
TITLE: A new method for the determination of N-terminal amino acids in polypeptides and proteins. III. Use of the reagent 2-chloro-3,5-dinitropyridine
AUTHOR(S): Signor, Angelo; Biondi, Laura; Terbojevich, Maria; Pajetta, Paola
CORPORATE SOURCE: Univ. Padua
SOURCE: Gazzetta Chimica Italiana (1964), 94(6), 619-29
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 61, 8611e. 2-Chloro-3,5-dinitropyridine (CA 59, 2811f) was found to react quant. with the N-terminal amino acids of proteins and peptides under relatively mild conditions to give the corresponding dinitropyridyl amino acids which were quant. recovered after acid hydrolysis. Further treatment of the dinitropyridyl amino acids with concentrated NH4OH gave the free amino acids. Approx. 1 μmol of dialyzed and dried protein was dissolved or suspended in a solution consisting of an equal weight of NaHCO3 and a 10-fold weight of H2O. Two vols. of an alc. solution of 2-chloro-3,5-dinitropyridine were added and the solution was agitated at room temperature for 2 h., then acidified with concentrated HCl, and extracted with EtOAc. The recovered dinitropyridyl-protein was dissolved in 1 mL. 98-100% HCOOH and hydrolyzed in 6N HCl for 15-30 min. at 100° or for 10-15 h. at 60°. The latter time and temperature conditions were required for maximum recovery of the dinitropyridyl derivs. of serine, threonine, and proline which undergo partial destruction. The hydrolyzates were diluted with H2O to pH 2 and extracted with 10-mL. portions of EtOAc. The several exts. were washed with 0.01N HCl and evaporated to dryness. The residue was dissolved in 5% NaHCO3 and again extracted, after acidification, with EtOAc. The resulting dinitropyridyl amino acids were determined by ascending and descending quant. two-dimensional paper chromatog. (Levy, CA 49, 101h; Biserte and Osteux, CA 45 7622g). The spots were localized under UV light, and were each cut out and extracted with 4 mL. 1% NaHCO3 at 60° for 30 min. After 10 min. at room temperature, the solns. were read at 340 mμ. The dinitropyridyl proline was read at 360 mμ. Data were obtained on the per cent amino acid liberated vs. hydrolysis time from the dinitropyridyl derivs. of 18 of the commonly occurring amino acids and glycylglycine, alanylglycine, alanylphenylalanine, and leucylleucine. It is concluded that the principal advantages of the method are in the relatively mild conditions of forming the dinitropyridyl-proteins and the stability of the dinitropyridyl amino acids during hydrolysis.
IT **2900-30-3**, Glycine, N-[1-(3,5-dinitro-2-pyridyl)-L-prolyl]-
3264-09-3, Proline, 1-(3,5-dinitro-2-pyridyl)-, L-
(in determination of amino acids in peptides)
RN 2900-30-3 HCAPLUS
CN Glycine, N-[1-(3,5-dinitro-2-pyridyl)-L-prolyl]- (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 3264-09-3 HCAPLUS
CN Proline, 1-(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 60 (Biochemical Methods)
IT 2578-45-2, Pyridine, 2-chloro-3,5-dinitro- **2900-30-3**,
Glycine, N-[1-(3,5-dinitro-2-pyridyl)-L-prolyl]- 2900-34-7,
Glycine, N-[N-(3,5-dinitro-2-pyridyl)-DL-alanyl]- 2900-36-9,
Glycine, N-[N-(3,5-dinitro-2-pyridyl)glycyl]- 3073-24-3,
Glutamic acid, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-25-4,
Isoleucine, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-26-5, Leucine,
N-(3,5-dinitro-2-pyridyl)-, DL- 3073-27-6, Serine,
N-(3,5-dinitro-2-pyridyl)-, DL- 3073-28-7, Threonine,
N-(3,5-dinitro-2-pyridyl)-, DL- 3073-29-8, Valine,
N-(3,5-dinitro-2-pyridyl)-, DL- 3264-06-0, Alanine,
N-(3,5-dinitro-2-pyridyl)-, DL- 3264-07-1, Alanine,
N-(3,5-dinitro-2-pyridyl)-3-phenyl-, DL- 3264-08-2, Glycine,
N-(3,5-dinitro-2-pyridyl)- **3264-09-3**, Proline,
1-(3,5-dinitro-2-pyridyl)-, L- 3426-97-9, Lysine,
N2,N6-bis(3,5-dinitro-2-pyridyl)-, L- 3521-73-1, Aspartic acid,
N-(3,5-dinitro-2-pyridyl)-, L- 19339-97-0, Glutamine,
N2-(3,5-dinitro-2-pyridyl)-, L- 91085-85-7, Asparagine,
N2-(3,5-dinitro-2-pyridyl)-, L- 92546-66-2, Arginine,
N2-(3,5-dinitro-2-pyridyl)-, L- 92872-58-7, Tryptophan,
N-(3,5-dinitro-2-pyridyl)-, L- 94063-05-5, Leucine,
N-[N-(3,5-dinitro-2-pyridyl)-DL-leucyl]-, DL- 94729-28-9,
Alanine, N-[N-(3,5-dinitro-2-pyridyl)-DL-alanyl]-3-phenyl-, DL-
(in determination of amino acids in peptides)

L26 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:462817 HCAPLUS
DOCUMENT NUMBER: 59:62817
ORIGINAL REFERENCE NO.: 59:11650h,11651a-c
TITLE: Structure of proteins. VII. Preparation of nitropyridylamino acids
AUTHOR(S): Signor, Angelo; Scoffone, Ernesto; Biondi, Laura
CORPORATE SOURCE: Univ. Padua, Italy
SOURCE: Gazzetta Chimica Italiana (1963), 93(1-2), 73-80
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 59:62817
AB cf. CA 59, 2811f. Adding 1.2 + 10-3 mole freshly prepared 2-

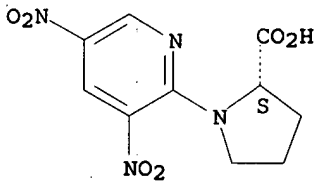
or 4-chloro-3,5-dinitropyridine in 40 cc. Me2CO to 10-3 mole amino acid in 30 cc. 5% aqueous NaHCO3, allowing the mixture to react 2-3 h. at ambient temperature with occasional stirring, evaporating solvent, diluting with H2O to the original volume, extracting with CHCl3, acidifying with 2N HCl to pH 2-3, filtering, and crystallizing from H2O or H2O-EtOH gave the 3,5-dinitro-4-(I)and 2-pyridylamino acids (II) in 80-98% yield, separated and identified by ascending paper chromatog. in 5:1:3:3 MePh-pyridine-Cl(CH2)2OH-0.8M NH3 and determined at 380-90 mμ for the 4-pyridyl and at 340 ± 2 mμ (except proline derivative 360 mμ) for the 2-pyridyl derivative (amino acid and m.p. of I and II given): glycine, 192°, 165°; DL-alanine, 185°, 164°; DL-serine, 225° (decomposition), 153°; DL-valine, 183°, 167°; L-leucine, 166°, 104°; L-tyrosine, 160°, 107°; DL-phenylalanine, 205°, 148°; L-proline, 150°, 157°; L-glutamic acid, 215° (decomposition), -; D-lysine, 113°, -. The stability of the derivs. under conditions of acid protein hydrolysis was determined by heating 5 + 10-5 mole 16 h. at 110° in closed vials in 1 cc. 6N HCl, evaporating HCl, bringing to pH 2.2 with citric buffer, diluting to 50 cc., and determining a 2-cc. sample on an automatic analyzer. II showed much greater stability than I; e.g. 3,5-dinitro-2-pyridylvaline hydrolyzed only 2%. 2-Chloro-3,5-dinitropyridine is recommended as a reagent for terminal amino acid determination

IT **3264-09-3**, Proline, 1-(3,5-dinitro-2-pyridyl)-, L-
(preparation of)

RN 3264-09-3 HCAPLUS

CN Proline, 1-(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 44 (Amino Acids, Peptides, and Proteins)

IT 3073-26-5, Leucine, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-27-6, Serine, N-(3,5-dinitro-2-pyridyl)-, DL- 3073-29-8, Valine, N-(3,5-dinitro-2-pyridyl)-, DL- 3264-06-0, Alanine, N-(3,5-dinitro-2-pyridyl)-, DL- 3264-07-1, Alanine, N-(3,5-dinitro-2-pyridyl)-3-phenyl-, DL- 3264-08-2, Glycine, N-(3,5-dinitro-2-pyridyl)- **3264-09-3**, Proline, 1-(3,5-dinitro-2-pyridyl)-, L- 82530-77-6, Glutamic acid, N-(3,5-dinitro-2-pyridyl)-, L- 89677-25-8, Glycine, N-(3,5-dinitro-4-pyridyl)- 89977-92-4, Alanine, N-(3,5-dinitro-4-pyridyl)-, DL- 89977-97-9, Serine, N-(3,5-dinitro-4-pyridyl)-, DL- 90871-34-4, Valine, N-(3,5-dinitro-4-pyridyl)-, DL- 93350-89-1, Leucine, N-(3,5-dinitro-4-pyridyl)-, DL-
(preparation of)

=> d que stat l31
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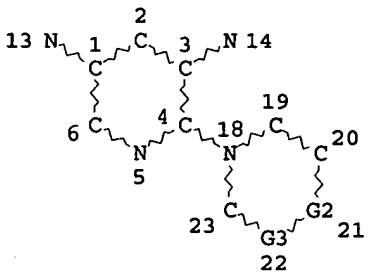

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STEREO ATTRIBUTES: NONE
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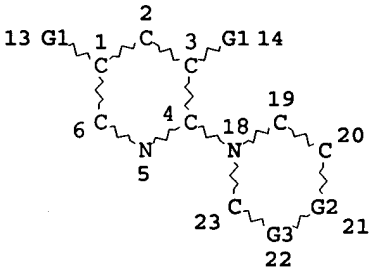

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DEFAULT MLEVEL IS ATOM
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NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
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L31 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:291093 HCAPLUS
DOCUMENT NUMBER: 140:326608
TITLE: New trinuclear heteroaromatic direct black dyes

INVENTOR(S): Kravtchenko, Sylvain; Lagrange, Alain; David, Herve; Greaves, Andrew; Bonaventure, Nicole; Vidal, Laurent
PATENT ASSIGNEE(S): L'Oreal, Fr.
SOURCE: Fr. Demande, 49 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2845387	A1	20040409	FR 2002-12385	20021004
FR 2845387	B1	20050121		
WO 2004031173	A1	20040415	WO 2003-FR2927	20031006
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003283499	A1	20040423	AU 2003-283499	20031006
US 2005060815	A1	20050324	US 2003-678635	20031006
EP 1551825	A1	20050713	EP 2003-775473	20031006
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.:		
FR 2002-12385	A	20021004
US 2002-431749P	P	20021209
WO 2003-FR2927	W	20031006

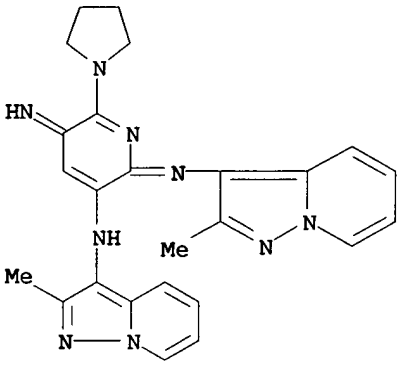
OTHER SOURCE(S): MARPAT 140:326608

AB New trinuclear heteroarom. direct dyes, the hair dye compns. containing these dyes as well as the process of dyeing of keratinous fibers are disclosed. The trinuclear heteroarom. direct black dyes comprise a pyridin core. The new dyes make it possible to obtain black nuances which have a good tenacity and stability in the hair dye compns. Thus, 3-amino-7-diethylaminopyrazolopyrimidine was reacted with 2-pyrrolidino-3-amino-6-methoxypyridine to obtain a trinuclear

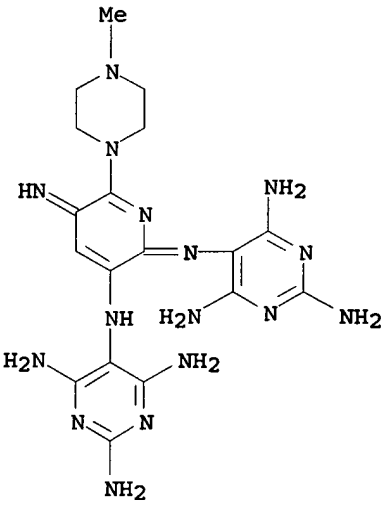
heteroarom. direct dye. Formulation of a dye containing 0.5% of above dye is disclosed.

IT **677314-81-7 677314-82-8 677314-83-9 677314-84-0 677314-85-1 677314-86-2 677314-87-3**
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(new trinuclear heteroarom. direct black dyes)

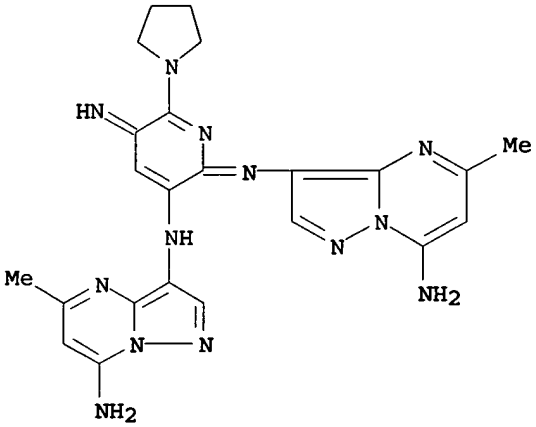
RN 677314-81-7 HCAPLUS
CN Pyrazolo[1,5-a]pyridin-3-amine, N-[2,5-dihydro-5-imino-2-[(2-methylpyrazolo[1,5-a]pyridin-3-yl)imino]-6-(1-pyrrolidinyl)-3-pyridinyl]-2-methyl- (9CI) (CA INDEX NAME)



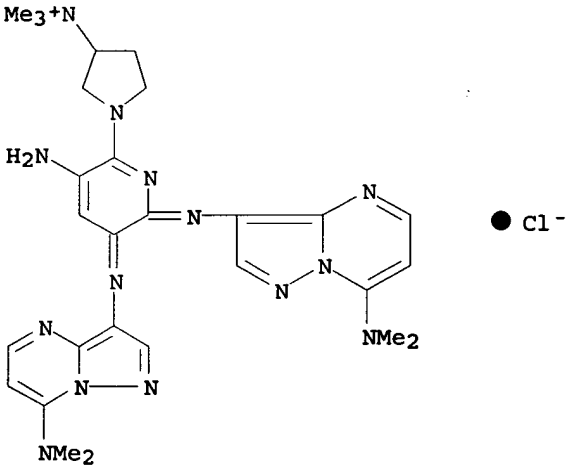
RN 677314-82-8 HCAPLUS
CN Pyrimidinetetramine, N5-[2,5-dihydro-5-imino-6-(4-methyl-1-piperazinyl)-2-[(2,4,6-triamino-5-pyrimidinyl)imino]-3-pyridinyl]- (9CI) (CA INDEX NAME)



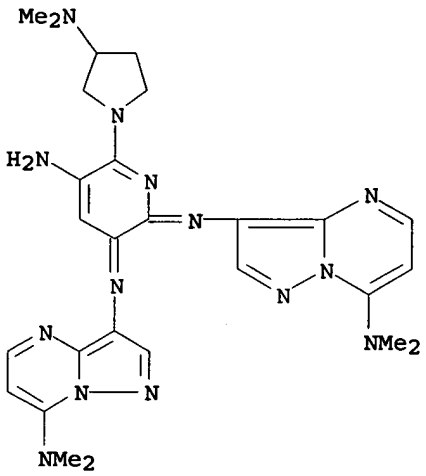
RN 677314-83-9 HCAPLUS
CN Pyrazolo[1,5-a]pyrimidine-3,7-diamine, N3-[3-[(7-amino-5-methylpyrazolo[1,5-a]pyridin-3-yl)amino]-5-imino-6-(1-pyrrolidinyl)-2(5H)-pyridinylidene]-5-methyl- (9CI) (CA INDEX NAME)



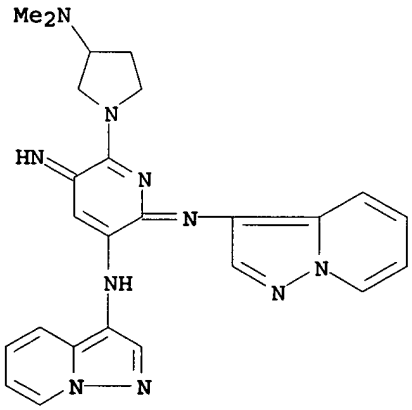
RN 677314-84-0 HCAPLUS
CN 3-Pyrrolidinaminium, 1-[3-amino-5,6-bis[[7-(dimethylamino)pyrazolo[1,5-a]pyrimidin-3-yl]imino]-5,6-dihydro-2-pyridinyl]-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



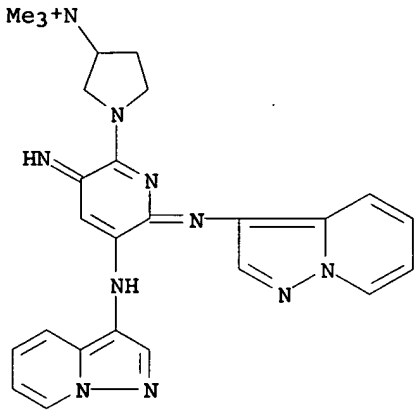
RN 677314-85-1 HCAPLUS
CN Pyrazolo[1,5-a]pyrimidine-3,7-diamine, N3,N3'-[5-amino-6-[3-(dimethylamino)-1-pyrrolidinyl]-2,3-pyridinediylidene]bis[N7,N7-dimethyl- (9CI) (CA INDEX NAME)



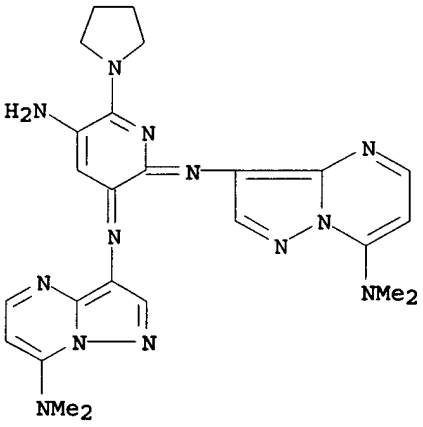
RN 677314-86-2 HCAPLUS
CN Pyrazolo[1,5-a]pyridin-3-amine, N-[6-[3-(dimethylamino)-1-pyrrolidinyl]-2,5-dihydro-5-imino-2-(pyrazolo[1,5-a]pyridin-3-ylimino)-3-pyridinyl]- (9CI) (CA INDEX NAME)



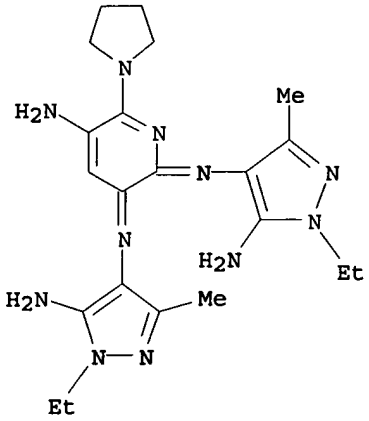
RN 677314-87-3 HCAPLUS
CN 3-Pyrrolidinaminium, 1-[3,6-dihydro-3-imino-5-(pyrazolo[1,5-a]pyridin-3-ylamino)-6-(pyrazolo[1,5-a]pyridin-3-ylimino)-2-pyridinyl]-N,N,N-trimethyl- (9CI) (CA INDEX NAME)



IT **677314-72-6P 677314-80-6P**
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(new trinuclear heteroarom. direct black dyes)
RN 677314-72-6 HCAPLUS
CN Pyrazolo[1,5-a]pyrimidine-3,7-diamine, N3,N3'-[5-amino-6-(1-pyrrolidinyl)-2,3-pyridinediylidene]bis[N7,N7-dimethyl- (9CI) (CA INDEX NAME)



RN 677314-80-6 HCAPLUS
CN 1H-Pyrazole-4,5-diamine, N4,N4'-[5-amino-6-(1-pyrrolidinyl)-2,3-pyridinediylidene]bis[1-ethyl-3-methyl- (9CI) (CA INDEX NAME)



IC ICM C07D471-04
ICS C07D401-14; A61K007-13; C07D231-38; C07D213-02; C07D239-42; C07D213-74; C07D209-40; C07D241-04; C07D213-90
CC 62-3 (Essential Oils and Cosmetics)
Section cross-reference(s): 28
IT **677314-81-7 677314-82-8 677314-83-9**
677314-84-0 677314-85-1 677314-86-2
677314-87-3 677314-88-4 677314-89-5
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(new trinuclear heteroarom. direct black dyes)
IT **677314-72-6P** 677314-74-8P 677314-75-9P 677314-76-0P
677314-77-1P 677314-78-2P 677314-79-3P **677314-80-6P**
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(new trinuclear heteroarom. direct black dyes)

L31 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:98457 HCAPLUS
DOCUMENT NUMBER: 134:147611
TITLE: Preparation of tetrahydrobenzo[d]azepines as metabotropic glutamate receptor 1 antagonists
INVENTOR(S): Adam, Geo; Binggeli, Alfred; Maerki, Hans-Peter; Mutel, Vincent; Wilhelm, Maurice; Wostl, Wolfgang
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: Eur. Pat. Appl., 85 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1074549	A2	20010207	EP 2000-116091	2000 0727
EP 1074549	A3	20020731		
EP 1074549	B1	20031119		
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AT 254614	E	20031215	AT 2000-116091	2000 0727
ES 2209728	T3	20040701	ES 2000-116091	2000

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CA 2314798	AA	20010206	CA 2000-2314798	
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US 6218385	B1	20010417	US 2000-630702	
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BR 2000003375	A	20010313	BR 2000-3375	
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PRIORITY APPLN. INFO.:			EP 1999-115557	A
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				0806

OTHER SOURCE(S): MARPAT 134:147611
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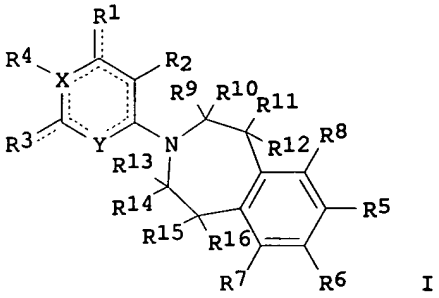
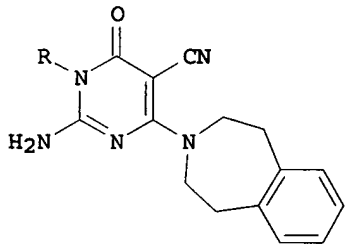


I



II

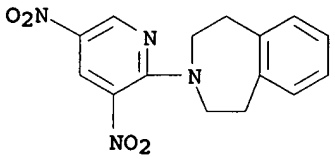
AB The title compds. (I) [wherein R1 = H, alkyl, O, halo, OR, cycloalkoxy, (un)substituted cycloalkylalkoxy, cyanoalkoxy, (fluoro)alkoxy, aminoalkoxy, alkenyloxy, phenylalkoxy, heterocyclylalkoxy, sulfonyloxyalkoxy, SR, carboxyalkylthio, NR2, hydroxyalkylamino, or heterocyclylalkylamino; n = 1-6; R = independently H, alkyl, or alkenyl; R2 = NO2 or CN; R3 = H, alkyl, O, S, SR, alkylsulfonyl, cycloalkyl, CONR2, NR2, alkyl, OR, or (un)substituted piperazino, carbamoylalkyl, alkoxyalkyl, fluoroalkyl, trifluoroacetoxyalkyl, carboxyalkyl, phenylthioalkyl, hetercyclylalkoxy, acylamino, alkylamino, phenoxyalkylamino, heterocyclylalkylamino, fluoroalkoxy, etc.; R4 = H, alkyl, alkenyl, NO2, OR, NR2, or (un)substituted fluoroalkoxy, fluoroalkyl, phenylalkyl, alkoxyalkanol, aminoalkyl, carboxyalkyl, alkylsulfonyloxyalkyl, fluoroalkenyl, heterocyclylalkyl, heterocyclylalkylamino, alkoxycarbonylamino, alkoxycarbonylhydrazino, aminofluoroalkenylamino; or R4 and R1 or R3 and R4 form an addnl. ring; R5 and R6 = independently H, alkyl, alkoxy, NH2, HO2, SO2NH2, or halo; or R5 and R6 = OCH2O; R7 and R8 = independently H, alkyl, alkoxy, NH2, NO2, or halo; R9 and R10 = independently H or alkyl; R11 and R12 = independently H, alkyl, OH, alkoxy, alkoxycarbonyloxy, or alkanoyloxy; R13 and R14 = independently H, T, or alkyl; R15 and R16 = independently H, T, alkyl, OH, alkoxy, alkoxycarbonyloxy, or alkanoyloxy; or R15 and R16 = O; X = N or C; Y = N, NH, or CH] were prepared For example, addition of Et 2-cyano-3,3-bis(methylthio)acrylate to 2,3,4,5-tetrahydro-1H-benzo[d]azepine•HCl using TEA and K2CO3 in EtOH gave 2-cyano-3-methylsulfanyl-3-(1,2,4,5-tetrahydrobenzo[d]azepin-3-yl)acrylic acid Et ester (64%). The benzazepinylacrylate ester was treated with NH2C(NH)NH2•HNO3 and 1,8-diazabicyclo[5.4.0]undec-7-ene in DMF to give II (R = H). Ethylation of II (R = H) with EtI in DMF in the presence of K2CO3 afforded the preferred metabotropic glutamate receptor 1 (mGluR1) antagonist II (R = Et), which gave an IC50 values of 0.009 μM and 0.003 μM, resp. in functional and binding assays for the characterization of mGluR1 antagonist properties. I are useful in the prevention or control of acute and/or chronic neurol. disorders and as radiolabeled mGluR1 receptor antagonists in binding assays (no data).

IT **324554-07-6P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tetrahydrobenzo[d]azepine mGluR1 antagonists by addition of chloroheterocycles or halobenzenes to tetrahydrobenzo[d]azepines or by cycloaddn. of guanidines to 3-methylthio-3-(tetrahydrobenzo[d]azepin-3-yl)acrylates)

RN 324554-07-6 HCAPLUS

CN 1H-3-Benzazepine, 3-(3,5-dinitro-2-pyridinyl)-2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



IC ICM C07D403-04
ICS A61K031-55; A61P043-00; C07D403-14; C07D401-04; C07D223-04; C07D405-14; C07D487-04; C07D401-14; C07F007-18; C07D471-04; G01N033-50

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT

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